Indian J. Phys. **74B** (6), 489–491 (2000)

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an international journal

Pseudo or quantal entropy—a signature of dynamical chaos

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Received 14 June 2000, accepted 24 August 2000

Abstract . A quantum pseudo or quantal entropy based approach has been used to study the onset of quantum chaos. Significant qualitative differences between chaotic and regular regime are demonstrated in the time evolution of pseudo entropy

Keywords Pseudo entropy, dynamical chaos

PACS No. 05 45 Mt

The presence of an irregular or chaotic regime in phase space of a dynamical system is of great importance in many areas of physics and chemistry [1] There are a number of several methods available to distinguish between regular and irregular motion [1,2]. Thus of great importance are methods that provide some, hopefully simple, predictions into the appearance of more widespread chaotic motion. The present communication attempts to explore such a possibility, by using pseudo or quantal entropy (S_Q) that has now often been used in the current literature in different contexts [3–5]

The Von-Neumann Shannon entropy of a pure quantum mechanical state is identically zero and remains so during its unitary evolution The quantum equivalent of thermodynamic entropy has therefore been of no help in understanding the emergence of quantum chaos

A theoretical construct, called the 'quantal' or pseudo entropy S_Q is as follows [3,4].

If one expands the statefunction $|\Psi\rangle$ in any orthonormal basis $|j\rangle$ as

$$|\Psi\rangle = \sum c_j |j\rangle \tag{1}$$

then S_Q (in dimensionless unit) is defined in the familier fashion–Tr $(\rho_d \ln \rho_d)$ where ρ_d is not the true density operator $|\Psi\rangle\langle\Psi|$, but just the diagonal part of it

$$(\rho_d)_{kl} = |c_k|^2 \delta_{kl} = \rho_{kk}\delta_{kl}. \tag{2}$$

Eq. (2) allows us to write

$$S_Q = -\sum |c_i|^2 \ln |c_i|^2 \tag{3}$$

This pseudo or quantal entropy (S_Q) has been found to have a global minimum under constraints It obeys the celebrated H-theorem and its constrained maximization yields a ground state wave function that satisfies virial theorem, the diagonal hypervirial theorem and so on [3,4]. However, it should be mentioned that this entropy is different from the conventional thermodynamic entropy in the sense that we have omitted the off-diagonal terms of the density operator. This may be viewed as coarse-grained version of the true thermodynamic entropy. Recently, we have studied the time evolution of the pseudo entropy of various model systems of physical and chemical interest and come to the conclusion that it has a characteristic signature of the dynamics of evolution of pure state under study [5].

In this communication, we demonstrate that the time evolution of the pseudo entropy as defined above, exhibits significant differences between regular and chaotic regimes in finite quantum systems

To illustrate the idea, we consider two examples

(1) A model system described by Pullen-Edmond (PE) Hamiltonian H_{PE} given by

$$\begin{aligned} H_{PE} &= \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{1}{2}\left(k_x x^2 + k_y y^2\right) + A x^2 y^2 \\ &= H_0 + A x^2 y^2 \end{aligned} \tag{4}$$

For the PE Hamiltonian, it is known [6] that for $A > 0.05$, all the trajectories with $E > 15$ are chaotic. Let us now consider the following situations. Suppose, we start from a highly excited eigenstate of H_0 and allow it to evolve adiabatically into the corresponding eigenstate of H_{PE}. The evolution is described by a time-dependent Hamiltonian $H(t)$ where

$$H(t) = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{1}{2}\left(k_x x^2 + k_y y^2\right) + \lambda(t) A x^2 y^2$$
$$= H_0 + \lambda(t) A x^2 y^2. \tag{5}$$

$\lambda(t)$ in eq. (5) is a switching function given by

$$\lambda(t) = \frac{t}{\tau} - \frac{\sin(2\pi t/\tau)}{2\pi}. \tag{6}$$

Now adiabatic switching from H_0 to H where the paremeter A in H has a value $A < 0.05$ corresponds to a transition between two regular Hamiltonians and the switching onto H having $A > 0.05$ corresponds to a transition from a regular to chaotic region. We follow the time evolution of S_Q during the switching process in these two cases by invoking the adiabatically switched time-dependent Fourier grid Hamiltonian method [7]. Figure 1(a) shows the time evolution of S_Q for the transition from a regular to a regular Hamiltonian and the Figure 1(b) is the same for the transition from a regular to chaotic Hamiltonian. One may note the considerable differences in S_Q *vs* t behaviour in these two cases.

(2) As a second example, we consider the Henon-Heiles Hamiltonian [8] given by

$$H = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{1}{2}\left(k_x x^2 + k_y y^2\right) - A\left(\frac{1}{3}x^3 - x^2 y\right)$$
$$= H_0 - A\left(\frac{1}{3}x^3 - x^2 y\right). \tag{7}$$

The Henon-Heiles system is a classic Hamiltonian which have been extensively used in the context of astronomy chemical dynamics over the last several decades [8–10]. This particular Hamiltonian shows regular behaviour for $A = 0.0$, for $A > 0.11864$ the system shows chaotic behaviour. As before, we consider two adiabatic transitions (i) one from H_0 to H (*cf.* eqn. 7) with the value of $A \ll 0.11864$, (ii) and the other from H_0 to H (*cf.* eq. 7) having A value > 0.11864. Figures 2(a) and 2(b) show the time evolution of S_Q in these two cases, respectively. From the figures, one may note a sharp differences in S_Q *vs* t profiles in two different regimes *viz.* switching from regular to regular and regular to chaotic region of the parameter space.

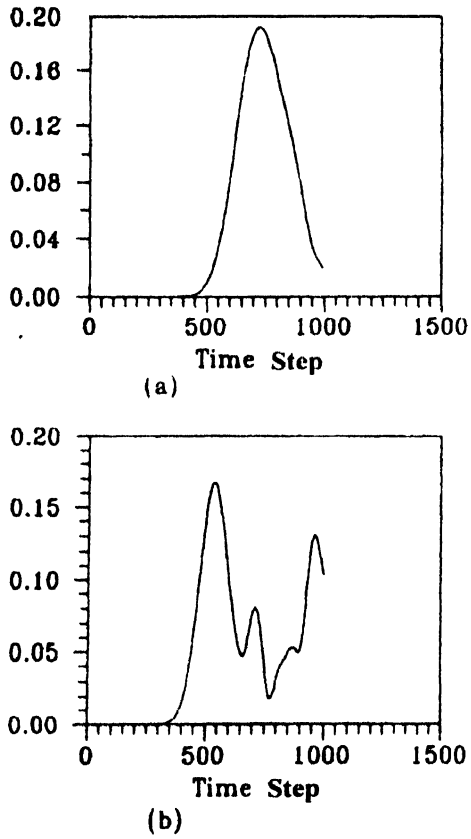

Figure 1. (a) The pseudo entropy *versus* time profiles of adiabatic evolution from a regular (Pullen-Edmond, $A = 0$) Hamiltonian to another regular Hamiltonian ($A = 0.02$) and (b) the same plot for an adiabatic transition from a regular Hamiltonian to a hamiltonian that generates quantum chaos ($A = 0.1$)

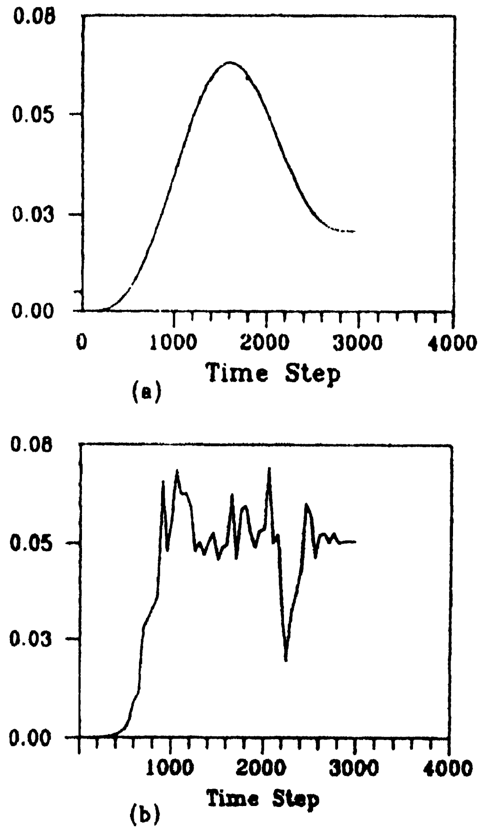

Figure 2. The pseudo entropy *versus* time profiles in two different regimes *viz.* (a) switching from a regular to a regular Henon-Heiles Hamiltoni. n ($A = 0.0524$) and (b) switching from regular to chaotic region of the parameter space ($A = 0.23728$)

In conclusion, we observe that the entropy S_Q defined in eq. (3) provides a useful tool for studying the onset of dynamical chaos in finite quantum systems. The difference between the time evolution of S_Q for fully developed chaotic and almost regular motion is striking and easily recognizable during adiabatic passage from a regular to chaotic regime.

Acknowledgments

The author would like to thank Prof. S P Bhattacharyya for some useful discussions.

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